Brief Announcement: Barrier-1 Reachability for Thermodynamic Binding Networks Is PSPACE-Complete

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Abstract

Chemical and molecular systems exist in a world between kinetics and thermodynamics. Engineers of such systems often design them to perform computation solely by following particular kinetic pathways. That is, just like silicon computation, these systems are intentionally designed to run contrary to the natural thermodynamic driving forces of the system. The thermodynamic binding networks (TBN) model is a relatively new model that is particularly well-equipped to investigate this dichotomy between kinetics and thermodynamics. The kinetic TBN model uses reconfiguration energy barriers to inform kinetic pathways. This work shows that deciding if two TBN configurations have a barrier-1 pathway between them is PSPACE-complete. This result comes via a reduction from nondeterministic constraint logic (NCL).

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1 Introduction and Preliminaries

The thermodynamic binding networks model, first presented in [5], was introduced in order to better study the connection between thermodynamic equilibrium and desired computational pathways. A TBN system, shown in Figure 1(Right), is simply a collection of monomer types which consist of complementary binding sites. Configurations of a TBN system are partitions of the monomers into polymers. A TBN configuration is said to be saturated if the bond count is maximized and said to be stable if it is saturated and the polymer count is maximized. Some recent work has been done on computing properties of stable configurations (i.e., at thermodynamic equilibrium) [3, 6]. Of particular interest to this announcement is the study of energy barriers along kinetic pathways in the TBN model [2] (described by merging and splitting polymers). In other words, how far away from equilibrium do these kinetic paths require the system to be (i.e., how many merges are required before a polymer may be split)? The *1-barrier reachability problem* states: Given two saturated TBN configurations, does there exist a saturated kinetic path between them with barrier at most 1? This announcement shows that this problem is PSPACE-complete by a reduction from constraint logic.

Constraint logic, shown in Figure 1(Left), is a very simple model where orientations are assigned to edges on a graph such that each vertex has minimum total inflow above a certain value (canonically inflow 2). Several questions have been studied in this model, but this announcement focuses on the nondeterministic constraint logic. The nondeterministic constraint logic (NCL) problem (a.k.a. *NCL configuration reachability*) asks if a goal configuration can be reached from an initial configuration through a sequence of edge

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orientation reversals such that no vertex's inflow constraint is ever unsatisfied. This problem was shown to be PSPACE-complete in [7]. Constraint logic has been used to show hardness for several problems including various games [7, 4], and motion planning [9, 1].

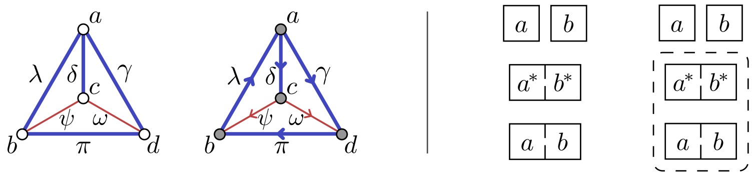

Figure 1 (Left) An example constraint graph $G = (V, E)$ (where $V = \{a, b, c, d\}$ and $E = \{\lambda, \delta, \gamma, \psi, \pi, \omega\}$) and satisfied state G_s. This graph consists of constraint-2 vertices, weight-2 edges (blue) and weight-1 edges (red). It is satisfied because all vertices have inflow of at least two. (Right) An example TBN $\mathcal{T}$and saturated (and stable) configuration S. The dotted-line box in configuration S indicates that monomers $\{a, b\}$ and $\{a^*, b^*\}$ are part of the same polymer (in this case, satisfying bonds a-a^* and b-b^*). S is saturated because all starred domains are bound (bonds are maximized), and it is stable because polymer count is maximized.

2 Complexity Result

Below is a brief explanation of how to transform a constraint graph into a TBN, followed by the outline for the PSPACE-completeness proof.

2.1 Transforming constraint graph into TBN

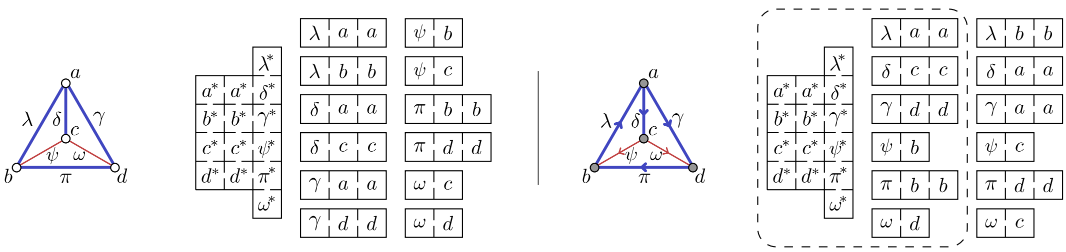

Figure 2 (Left) An example constraint graph G and corresponding TBN $\mathcal{T}$. (Right) Satisfied state G_s and corresponding saturated configuration S.

Figure 2 illustrates the technique for constructing a TBN given a constraint graph. The primary idea is to construct two "types" of monomers: (1) a *constraint monomer* in the TBN which contains one starred domain per edge and two starred domains per vertex in the constraint graph and (2) two *edge monomers* per edge in the constraint graph (for each edge direction), each with an edge domain and vertex domain(s) dictated by edge weight. It should be noted that this reduction allows for a rather simple proof that a TBN constructed in this way has a saturated configuration with at least $|E| + 1$ polymers if and only if the given constraint graph is satisfiable (both previously know NP-complete problems shown in [3] and [7], respectively).

2.2 Barrier-1 Reachability is PSPACE-complete

Figure 3 is provided as a visual aid to accompany the intuition given in the proof sketch.

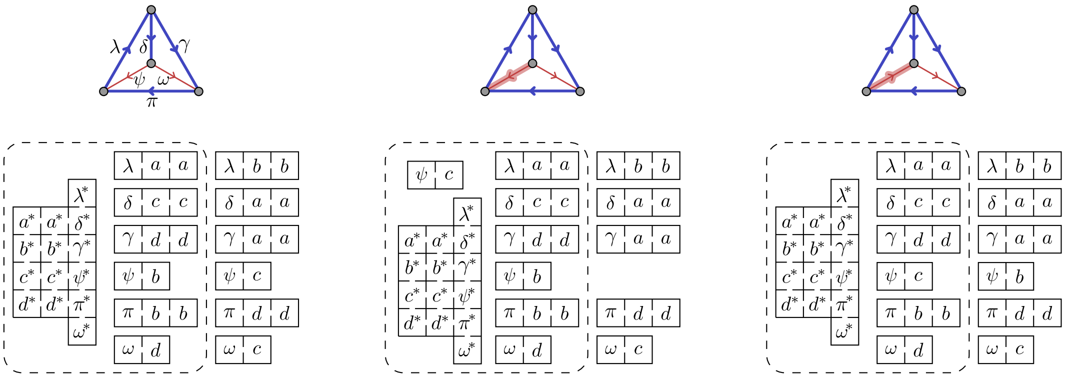

Figure 3 An example constraint logic edge flip along with the equivalent TBN merge/split path.

▶ **Theorem 1.** *The 1-barrier reachability problem is PSPACE-complete.*

A sketch of the proof is as follows: PSPACE-hardness is shown via a reduction from nondeterministic constraint logic reachability. Specifically, there exists a barrier-1 kinetic path between two saturated configurations in the TBN if and only if there exists a valid move sequence between the satisfied constraint logic configurations. The key idea is that a satisfied constraint logic state is represented by a stable TBN configuration with $|E| + 1$ polymers, and a valid edge flip can be simulated by single merge followed by a split operation in the TBN while invalid edge flips require at least two sequential merges. The converse is proven similarly. A simple argument then shows membership in NPSPACE which, by Savitch's theorem [8], means the problem is in PSPACE and thus PSPACE-complete.

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